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Unraveling the Symmetry of Hole States in the MgB_2 Superconductor

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Beamline(s): U7A

Introduction: We combine x-ray absorption spectroscopy (XAS) at U7A and electron energy loss spectroscopy in an electron microscope to study at room temperature the near edge fine structure of MgB_2 at the K-edge of boron. We observe in the XAS study of a polycrystalline sample a peak of width 0.7 eV at the threshold of the K-edge, signaling a narrow energy region with empty boron p-states near the Fermi level. In the electron microscope (TEM), an individual crystallite, or even part of a crystallite, can be isolated with a focussed beam. Changes in near edge structure observed in EELS with changes in direction of the momentum transfer between incident electrons and the crystal show that these states have primarily p_xp_y symmetry. Our observations are consistent with electronic structure calculations indicating a narrow energy window of empty p_xp_y states that falls to zero 0.8 eV above the Fermi level. The absence of the p_xp_y feature in EELS spectra from grain boundaries suggests that this signature may be a crucial indicator of superconducting properties at the nanoscale.

Methods and Materials: Several MgB2 polycrystalline samples were prepared at BNL. The XAS spectra were obtained at U7A NSLS using an energy sweep with 0.05 eV steps chosen to approximate the energy resolution. The EELS measurements were obtained with a 300 keV JEOL 3000F TEM equipped with a field emission gun, using a focussed beam as fine as 1 nm. Analysis of EELS data entails background subtraction and a correction for multiple scattering not necessary in the case of XAS.

Results: The main feature of the K-edge of boron is a peak of width ~0.7 eV at the edge threshold, 186.5 eV (Fig.1). Similarly sharp peaks at 191.5 and 193.5 eV are attributed to boron nitrides and oxides respectively. EELS measurements of crystallites provides specific directional information. We find that the 186.5 eV peak corresponds predominately to p_xp_y states, with less weight from the p_z states. Using the ~1 nm EELS probe, with a large convergence angle to wash out the angle dependence, it is also possible to study the differences between the interior of a grain and its exterior. The p_xp_y states near 186.5 eV are noticeably suppressed near the grain boundary.

Conclusions: This study of the boron K-edge in MgB_2 is consistent with the results from electronic structure calculations. We observe pxpy boron states up to 0.8 eV above the Fermi level. Our observations support the conjecture that superconductivity in MgB2 is driven by the $\sigma(sp_xp_y)$ band holes.

Reference: Y. Zhu, et al. submitted.

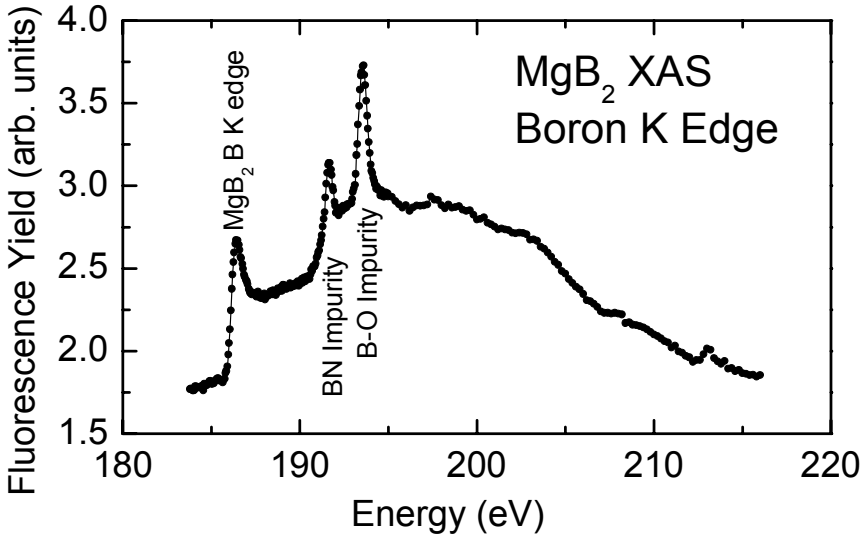

Figure 1. Boron K edge for polycrystalline MgB_2 obtained at NSLS beamline U7A illustrating the sharp prepeak at 186.5 eV as well as prominent impurity peaks identified with boron nitrides and oxides. In the case of EELS in the TEM, the fine focus of the beam onto a single crystallite eliminates potential impurity signals.